Theory of integer quantum Hall effect in bilayer graphene near neutrality point

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A Hartree-Fock variational ground state for dual-gated bilayer graphene (BLG) in the presence of magnetic fields is proposed. We argue that near the charge neutrality point (CNP), a Néel as well as uniform magnetization can coexist in the presence of the magnetic fields. An infinitesimal Zeeman coupling restricts the Néel order to the easy plane and develops magnetization in the direction of the field. Many-body effects further enhance the size of the magnetization. Such interaction induced gap near the CNP displays a quadratic dependence with the field, when it is weak. It then crosses over to a linear one at intermediate strength of the field, and possibly persisting even at stronger fields. These features are in qualitative accordance with a recent experimental observation. Furthermore, with realistic strengths of the interactions, we establish an *quantitative* agreement with experiment for 0 T < B < 4.5 T. Upon tilting the field, the Néel order gradually vanishes and a pure ferromagnetic order emerges beyond a critical strength of the *total* field, which otherwise depends monotonically on its perpendicular component and the zero field gap. Formation of additional incompressible Hall states and the nature of the broken symmetry phases at other fillings, e.g., $\nu = \pm 2$, are discussed as well.

Introduction: Nature of the underlying broken symmetries in quantum Hall systems has recently been an active field of research following the successful realization of the carbon-based layered materials, for example mono-layer graphene (MLG) and BLG. They respectively discern quantized plateaus of Hall conductivity at fillings $\nu = \pm(4n + 1)$ and $\pm(4n + 2)$, at relatively weak magnetic fields [1]. The four fold degeneracy of each Landau levels (LLs) arises from the spin and the valley degrees of freedom. The additional orbital degeneracy of the zeroth LL in BLG, bears the signature of the quadratic quasiparticle dispersion around the Dirac points, opposed to the linear ones in MLG [2, 3]. The distinct topologies of such simple band structures leave profound impacts on the role of electron-electron interactions in those systems. Weak electron-electron interactions are *irrelevant* in MLG [4], while they can cause various instabilities in BLG [5]. The nature of the broken symmetric phases in BLG, is however sensitive to the range of interactions. A weak coupling renormalization group calculation predicts that BLG can be found either in metallic *nematic* or insulating antiferromagnet (AF) phases, when interaction is respectively long and short-ranged [6, 7]. In recent experiments, the nematic [8] as well as an insulating [9] phase has been observed, in the presence of single and dual gate, respectively. For simple onsite Hubbard model, the most dominant instability is towards the formation of a staggered pattern of spin among the layers, the AF phase [10].

In a half-filled bipartite lattice, for example BLG, the Stoner instability towards the formation of a ferromagnet (FM) order is preempted by the appearance of an AF phase. Therefore the double-gated BLG is gapped, possibly with an AF order. However, in the presence of magnetic fields, even an infinitesimal Zeeman coupling can modify the nature of the ordered phase. It projects the Néel order onto an easy plane, and concomitantly favors a magnetization in direction of the field, which unless otherwise mentioned is set to be perpendicular to the BLG plane. Many body effect further enhances the size of the magnetization. A similar ground state has also been proposed recently for neutral MLG subject to quantizing magnetic fields [11]. A recent experiment [9], discerns a gap $(2\Delta_0) \sim 1$ meV in dual-gated BLG in the absence of the field at the CNP $(\nu = 0)$, which otherwise increases monotonically with the magnetic field (B), and closely resembles to the form

$$E_{gap} = \Delta_0 + \sqrt{\Delta_0^2 + a^2 B^2}, \qquad (1)$$

where $a = 5.5$ meV/T. Therefore, at low fields E_{gap} gap varies quadratically with the field, which then reverts to a linear one at stronger fields. Dependence of the gap in the presence of on weak electric field, applied perpendicular to the BLG, rules out the possibility of a layer polarized state, corresponding to an imbalance of average electronic density among the layers [12, 13]. Here we analyze the scaling behavior of the above proposed ordered phase with the field. We show that developing a sizable magnetization in the direction of the field, a quantitative agreement with the experiment can be established, at least when the field is weak.

The ground state: Hereafter we assume a uniform background of electronic density and Néel $(\vec{N})$ order as well as magnetization $(\vec{M})$ in the BLG system. The ground state energy per unit area of the BLG at half-filling can therefore be written as [14]

$$E_{gr} = \frac{\vec{N}^2}{4g_A} + \frac{\vec{M}^2}{4g_F} + E_0\left[\vec{N}, \vec{M}\right]. \qquad (2)$$

$E_0\left[\vec{N}, \vec{M}\right]$ is the ground state energy per unit area of

the effective single-particle Hamiltonian

$$H_{HF} = I_2 \otimes H_0 - \left(\vec{N} \cdot \vec{\sigma} \right) \otimes \gamma_0 + \left(\lambda + M \right) \sigma_3 \otimes I_4, \quad (3)$$

where

$$H_0 = \gamma_2 \left(\frac{\pi_x^2 - \pi_y^2}{2m^*} \right) + \gamma_1 \left(\frac{-\pi_x \pi_y - \pi_y \pi_x}{2m^*} \right). \quad (4)$$

$m^* \approx 0.033 m_e$ is the effective mass of the parabolic dispersion around two inequivalent Dirac points $\pm \vec{K}$, with $\vec{K} = \left(1, 1/\sqrt{3} \right) \left(2\pi/a\sqrt{3} \right)$ [8]. m_e is the mass of ordinary electrons and a is the lattice spacing of the underlying honeycomb lattice in each layers. $\pi_j = \left(-i\partial_j - A_j \right)$, with $j = x, y$ and we set the magnetic field (B) to be perpendicular to the BLG plane, i.e., $B = \epsilon_{3ij} \partial_i A_j$. Therefore the magnetization is kept only in the direction of the field, $\vec{M} \equiv M\hat{z}$. $\lambda = \lambda_Z \omega_c$ is the Zeeman coupling, where ω_c is the cyclotron frequency and $\lambda_Z \approx 0.015$ for BLG. H_{HF} is written in a rotationally invariant basis $\Psi = \left(\Psi_\uparrow, \Psi_\downarrow \right)^\top$, where $\Psi_\sigma^\top =$

$$\left[v_{1,\sigma}(\vec{K} + \vec{q}), v_{2,\sigma}(\vec{K} + \vec{q}), v_{1,\sigma}(-\vec{K} + \vec{q}), v_{2,\sigma}(-\vec{K} + \vec{q}) \right].$$

$\sigma = \uparrow, \downarrow$ corresponds to the projections of spin along the z-direction. $i = 1, 2$ corresponds to two layers of BLG. The mutually anti-commuting four component Hermitian gamma matrices are $\gamma_0 = \sigma_0 \otimes \sigma_3, \gamma_1 = \sigma_3 \otimes \sigma_2, \gamma_2 = \sigma_0 \otimes \sigma_1, \gamma_3 = \sigma_1 \otimes \sigma_2, \gamma_5 = \sigma_2 \otimes \sigma_2$ [15]. The spectrum of H_{HF} is therefore comprised of a set of Landau levels at well separated $\pm e_{n,\sigma}$, where

$$e_{n\sigma} = \left[N_\perp^2 + \left(\left[n(n-1)\omega_c^2 + N_\parallel^2 \right]^{1/2} + \sigma \left(\lambda + M \right) \right)^2 \right]^{1/2}, \quad (5)$$

with $\vec{N}_\perp = (N_1, N_2), N_3 \equiv N_\parallel$ and $\sigma = \pm 1$, with degeneracies per unit area $1/\pi l_B^2$ for $n = 2, 3, 4, \cdots$ and $1/2\pi l_B^2$ for $n = 0, 1$ [16]. $l_B = \sqrt{(\hbar c/eB)}$, is the magnetic length. At half-filling, all the states at negative (positive) energies are filled (empty). Therefore,

$$E_0 \left[\vec{N}, M \right] = -\frac{1}{2\pi l_B^2} \sum_{\sigma = \pm} \left(e_{0\sigma} + e_{1\sigma} + 2 \sum_{n \geq 2} e_{n\sigma} \right). \quad (6)$$

To find the configuration of $\vec{N}$ to minimize the Hartree-Fock ground state energy, we choose $|\vec{N}|$ and $N_\parallel$ as independent variables. Then $\partial E_0 \left[\vec{N}, M \right] / \partial N_\parallel = 0$ yields

$$\sum_{\sigma = \pm} \sigma \left(\lambda + M \right) \left[\sum_{n=0,1} \frac{1}{e_{n\sigma}} + \sum_{n \geq 2} \frac{2N_\parallel}{e_{n\sigma} \sqrt{N_\parallel^2 + n(n-1)\omega_c^2}} \right]$$

$$= 0. \quad (7)$$

The left hand side of this equation is negative definite function of $N_\parallel$ and vanishes only for $N_\parallel \equiv 0$. Therefore, in the presence of even infinitesimal Zeeman coupling the Néel order is projected onto the easy plane ($N_\parallel = 0$), perpendicular to the direction of the magnetic field. This configuration also corresponds to the minima of the energy. An identical ground state has also been proposed for MLG previously [11]. Therefore, in the presence of the field, the total gap at charge-neutrality point ($\nu = 0$) is

$$E_{gap}(\nu = 0) = \sqrt{N_\perp^2 + (\lambda + M)^2}. \quad (8)$$

Next we find the self consistent solution of $|\vec{N}_\perp|$ and M as a function of the magnetic fields.

Gap equations: One can now arrive at the self consistent gap equations by minimizing E_{gr} w.r.t the Néel and the magnetization orders, separately. After some tedious otherwise straightforward algebra, in terms of a new set of variables $\delta_N = N_\perp/\Delta_0, \delta_m = M/\Delta_0, \beta = \omega_c/\Delta_0$, the minimization of E_{gr} w.r.t. $N_\perp$ and m respectively yield, either $\delta_N = 0$ or

$$\frac{2}{g_A} = \sum_{\sigma = \pm 1} \int_{\frac{\sqrt{3}}{2}}^{\Omega} \frac{\xi d\xi}{X(\xi, \delta_N, \delta_m, \lambda, \beta, \sigma)} + \frac{2\beta^2}{\sqrt{\delta_N^2 + \beta^2 y^2}} \quad (9)$$

and $\delta_m = 0$ or

$$\frac{2\delta_m \beta^{-1}}{g_F} = \sum_{\sigma = \pm 1} \int_{\frac{\sqrt{3}}{2}}^{\Omega} \frac{(\sigma \xi^2 + y\xi) d\xi}{X(\xi, \delta_N, \delta_m, \lambda, \beta, \sigma)} + \frac{2y\beta^2}{\sqrt{\delta_N^2 + \beta^2 y^2}}, \quad (10)$$

taking $8g_{A,F}/2\pi \to g_{A,F}$ [17]. Here $y = \lambda_Z + \delta_m \beta^{-1}$, and

$$X(\xi, \delta_N, \beta, y) = \sqrt{\xi^2 + \frac{1}{4}} \sqrt{\frac{\delta_N^2}{\beta^2} + [\xi + \sigma y]^2}. \quad (11)$$

In last two equations we neglect the contributions, not relevant at low fields, i.e., $\beta \ll 1$. As the ultra-violet cut-off $\Omega \to \infty$ the right-hand side of Eq. [9] exhibits a logarithmic divergence, whereas the next equation is completely divergence free. Such an outcome is directly related to the LL spectrum in Eq. [5]. The AF order and magnetization, respectively shift and split all the LLs at finite energies, whereas both develop gap within the zeroth LL. A similar spectrum of the LLs is found in MLG [11]. To ensure the cut-off independence of the order parameters, we substitute

$$\frac{1}{g_A} = \int_0^\Omega \frac{d\xi}{\sqrt{\xi^2 + \Delta_0^2}} \equiv \int_0^{\frac{\Omega}{\Delta_0}} \frac{d\xi}{\sqrt{\xi^2 + 1}}. \quad (12)$$

in Eq. [9], where Δ_0 is the zero field gap of the Néel order. On the other hand, g_F remains as a free parameter. To evaluate the right-hand-side of the gap equations we reformulate them by using the *Feynman parametrization* [18]

$$\frac{1}{\sqrt{AB}} = \frac{1}{\pi} \int_0^1 \frac{dy}{\sqrt{y(1-y)}} \left[\frac{1}{yA + (1-y)B} \right]. \quad (13)$$

One can then perform the integrals by using the "Euler substitution" [19]. In this prescription, we manage to evaluate all the divergent integrals analytically. The remaining finite integrals are computed numerically.
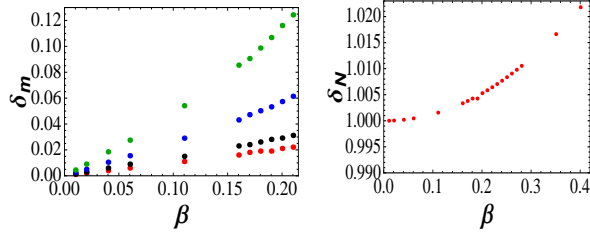

FIG. 1: Left: Magnetization ($\delta_m = M/\Delta_0$) in neutral BLG for $g_F = 0.58$ (red), 0.6 (black), 0.63 (blue), 0.65 (green). Right: AF ($\delta_N = N_\perp/\Delta_0$) order for $g_F = 0.58$. Here $\beta = \omega_c/\Delta_0$

Numerical strategy: To find the self-consistent solutions of two order parameters, we here pursue the following numerical approach. For each field strength, first we find the zeros of the Eq. [9] in the (δ_N, δ_m) plane, yielding a closed curve. Taking the ansatz $\delta_N = \tan\theta \, \delta_m$, corresponding to a family of rays passing through the origin otherwise enjoying intersections with that closed curve, we compute only positive roots (i.e., $0 \leq \theta \leq \pi/2$) of Eq. [9]. Plugging these roots in Eq. [10], we search for the self-consistent solutions of δ_N and δ_m, for various values of g_F.

Scaling: The AF order is finite at zero field and grows quadratically with the field, if the field is weak ($\beta \ll 1$). The curvature of the quadratic variation of the AF order decreases with increasing g_F, though not considerably. The magnetization, on the other hand, varies linearly with the field, but vanishes in its absence. As g_F increases, magnetization is enhanced. This features are depicted in Fig. [1]. Hence to the leading order, the gap near the CNP $E_{gap}(\nu = 0)$ scales quadratically with the field, when it is weak, as expected from Eq. [8]. The scaling of the total gap in the weak field limit for $g_F = 0.6$ is shown in left column of Fig. [2]. A similar qualitative picture has been attained previously considering only an AF order. However, the curvature is *four* times smaller than the observed one [6]. As g_F gets stronger, the curvature of the scaling function increases, shown in right column of Fig. [2]. The coefficient of the quadratic term are found to be 0.13, 0.17, 0.25, 0.45 respectively for $g_F = 0, 0.6, 0.63, 0.65$ from numerical fitting. For smaller $g_F(< 0.5)$ the curvature does not change considerably from the one with a pure AF order, i.e., $g_F \equiv 0$. To establish the connection of our result with the recent experiment [9], one must take into account that the zero field gap in Eq. [1] is $2\Delta_0$ [9], while in our analysis it reads as Δ_0. The coefficient in front of β^2 in the scaling of interaction induced gap at $\nu = 0$, is then found to be 0.5 in experiment, while that for $g_F = 0.65$ gives 0.45 from a numerical fitting, see Fig. [3]. Therefore by developing a finite magnetization, $\sim (10^{-3} - 10^{-4})\mu_B$ per

electron when $B \sim 1$ T, where μ_B is Bohr magneton, the quadratic scaling of the interaction induced gap in weak fields, is found in reasonable agreement with the experiment [9, 20]. On the other hand, at intermediate strength of the field ($\beta \geq 0.6$ for $g_F = 0.65$) the gap starts to deviate from the quadratic variation, and enters the regime of a linear variation with the field, shown in Fig. [3]. The field strength associated with such crossover reduces with increasing g_F. However, the slope of the linear scaling function remains close to the one found previously for a pure AF state. To be precise, the slope of the scaling function increases slightly, though it is still off by a factor of 1.85 from the observed one. The same quantity for a pure AF gap is found to be off by a factor 2 [6].

The role of the single-particle Zeeman coupling, even though small, is crucial. We also compute the self consistent solution of δ_N and δ_m, setting $\lambda \equiv 0$. A non-trivial magnetization then develops only for $g_F > 3$. The Stoner instability from $\vec{N}_\perp \neq 0, m = 0$ to $\vec{N}_\perp \neq 0, m \neq 0$ phase, is possibly a *weak first order transition*.

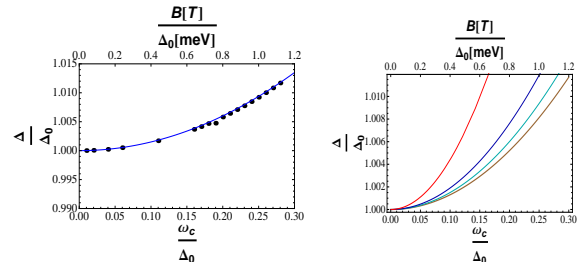

FIG. 2: Left: total gap at CNP for $g_F = 0.6$. Black dots are numerical solutions and blue one is the quadratic fit of the gap with the field. Right: total gap at CNP for $g_F = 0$(brown), 0.6(cyan), 0.63(blue), 0.65(red)

Discussion: To summarize, we show that by developing a sizable magnetization in the direction of the field, while restricting the Néel order into easy plane one can explain the observed scaling of the interaction induced gap near CNP in double-gated BLG, at least when the field is weak. At moderate field strengths the scaling of the interaction induced gap appears to crossover to a linear regime, which possibly persists even for stronger fields. However, the slope of the linear scaling is off by an factor of 1.85 from the experiment. The reason for such mismatch is not clear, although it may arise due to the existence of additional OPs in high fields. Within the zeroth LL, the quantum spin Hall insulator is exactly proportional to the magnetization. The electron-electron interactions can therefore develop the spin Hall order at stronger fields, when the LL quantization is sharp. Yet another order, pointed out by Kharitonov [21], preserving the layer inversion symmetry, odd under the exchange of Dirac points, and breaks spin rotational symmetry, can coexist with the AF order within the zeroth LL. Otherwise, it scales linearly with the field and vanishes in its absence. Therefore, developing a sizable component of this order one can meet the slope at high fields, observed

experimentally. However, such an order commutes with the AF order, unlike the FM order. Therefore existence of such order cannot change the curvature of the gap from the one with pure AF phase, at weak fields.
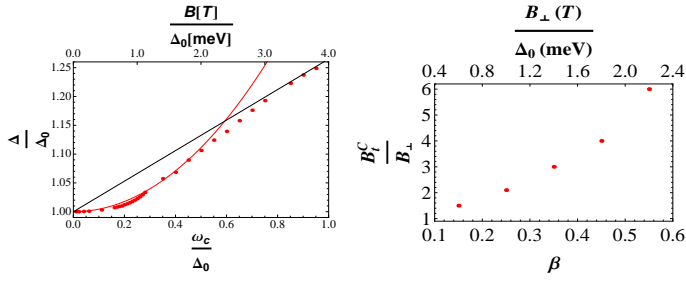

FIG. 3: Left: Total gap at CNP as a function of the field $0 < B(\mathrm{T}) < 4.5$ for $g_F = 0.65$. Red dots are numerically found solutions, whereas the solid lines are fitting functions. Right: Critical total field ($B_t^C/B_\perp$) for various strength of perpendicular field ($B_\perp$), necessary to destroy the AF order at CNP.

Validity of the proposed scenario can be tested by placing the dual-gated BLG in tilted magnetic fields. AF order scales with the perpendicular component of the field ($B_\perp$), while the magnetization scales with the total magnetic field (B_t). With increasing B_t but a fixed $B_\perp$, the Néel order gradually decreases, whereas the FM order increases with B_t and beyond a critical total field (B_t^C), system can be found in a pure FM phase. With $g_F = 0.65$, we here compute B_t^C for various $B_\perp$, shown in the right column of Fig. [3]. It is evident that for stronger $B_\perp$, B_t^C gets larger, due to the monotonic increment of AF order with $B_\perp$. Otherwise, B_t^C scales quadratically with $B_\perp$, revealing the quadratic variation of AF with $B_\perp$, shown in Fig. [1]. With zero field gap $\Delta_0 = 1.13$ meV as in Ref. [9], $B_t^C \approx 1.02, 2.4, 4.8, 8.1, 15$ T respectively for $B_\perp = 0.68, 1.13, 1.6, 2.03, 2.5$ T. In experiment, one can increase B_t while keeping $B_\perp$ fixed by tilting the BLG sample, where the tilting angle reads as $\theta_t = \cos^{-1}(B_\perp/B_t)$. For a fixed $B_\perp$, B_t^C is lowered if the zero field gap (Δ_0) gets smaller. For example, with $B_\perp = 1.6$ T, $B_t^C = 4.8, 3.8, 2.95$ T for $\Delta_0 = 1.13, 0.9, 0.7$ meV, respectively, if $g_F = 0.65$. In dual-gated BLG, one can reduce the size of the zero field gap by applying a weak electric field among the two layers [13]. Appearance of such pure FM phase can be confirmed by measuring the longitudinal resistivity R_{xx} [22]. The field induced FM phase can host counter propagating edge modes of opposite spin polarity, similar to MLG [23], hence R_{xx}

becomes much smaller than that in presence of a Néel order.

Placing the chemical potential close to the first excited state at $\pm E_{gap}(\nu = 0)$, additional incompressible Hall states at filling $\nu = \pm 2$ can be formed by developing a third component of the Néel order ($N_3 \equiv N_\parallel$), parallel to the applied magnetic field. To the linear order in N_3 the activation gap for $\nu = \pm 2$ reads as

$$E_{gap}(\nu = \pm 2) = 2\frac{\lambda + M}{\left(N_\perp^2 + (\lambda + M)^2\right)^{1/2}}N_3 + \mathcal{O}(N_3^2).$$

(14)

Similarly, in MLG, the $\nu = \pm 1$ Hall states can also be formed by developing N_3 [11]. The scaling of the $\nu = 1$ state in MLG, has been computed for large number of fermionic species [24]. The component of Néel order in the direction of the field arises only from the zeroth LL, whereas its easy plane component is finite in all the LLs. Therefore $N_3 \sim B$, whereas $M \sim B$ and $(N_\perp(B) - \Delta_0) \sim B^2$, at least when the field is weak. Therefore the gap for $\nu = \pm 2$ Hall state is expected to scale quadratically with weak fields, otherwise vanishes at zero field. The coefficient of the term proportional to B^2 in Eq. [14] scales as $1/\sqrt{\Delta_0}$. Therefore curvature of the activation gap of $\nu = \pm 2$ state in weak fields is expected to increase upon applying a weak electric field between the layers, which decreases the size of the zero field gap [13]. On the other hand, in the presence of a strong tilted field, when $N_\perp = 0$, activation gap for $\nu = \pm 2$ Hall state scales linearly with the field. A simple estimation yields that for weak fields $B < 10$ T, $N_3 \sim (a/l_B)^2\mu_B \sim (10^{-3} - 10^{-4})\mu_B$ per electron, similar to that in MLG [11]. Measurement of such a small component of the Néel order at $\nu = \pm 2$, can test the validity of the nature of broken symmetry phases in BLG subject to magnetic fields.

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